Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 10.3 days

Global applicability domain: Inside

Local applicability domain index: 6.15e-01

Confidence level: 6.39e-01

Nearest Neighbors from the Training Set

Image not found
Benzene
Measured: 61.9
Predicted: 10.3

Image not found
Cyclohexane
Measured: 8170
Predicted: 34.7

Image not found
Cyclopentane
Measured: 8170
Predicted: 35.5

Image not found
1,2,4,5-Tetramethylbenzene
Measured: 88.3
Predicted: 5.46

Image not found
Biphenyl
Measured: 2720
Predicted: 17.6